Supporting information for

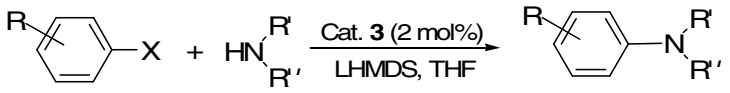
Alkylpalladium *N*-Heterocyclic Carbene Complexes: Synthesis, Reactivity and Catalytic Properties

Oriana Esposito,[a] Pedro M. P. Gois,[a,b,c] Alexandra K. de K. Lewis,[c] Stephen Caddick,[c]* F. Geoffrey N. Cloke[a]*

[a] Department of Chemistry and Biochemistry, School of Life Sciences, University of Sussex, Falmer, Brighton BN1 9QJ, UK; [b] CQFM, Departamento de Engenharia Química e Biologia, Complexo I, Instituto Superior Técnico, Av. Rovisco Pais 1, 1049-001 Lisboa, Portugal; [c] Department of Chemistry, University College London, 20 Gordon Street, London WC1H OAJ, UK;

Email Address: s.caddick@ucl.ac.uk; f.g.cloke@sussex.ac.uk

Scope of Buchwald-Hartwig amination reactions using complexes **3 – Scheme 8, Table 2**



General procedure for the Buchwald-Hartwig cross-couplings (Scheme 8, table 2).

In a glovebox, to a round bottom flask equipped with a magnetic stir bar was added the palladium precatalyst (2 mol%) and the base (0.456 mmol, 1.3 eq), after which the flask was closed with a septum and taken out off the glovebox. Dry THF (0.5 mL), amine (0.421 mmol, 1.2 eq) and aryl halide (0.351 mmol) were than sequentially add trough the septum. The reaction mixture was than stirred at room temperature unless otherwise indicated. When the reaction reached completion (the disappearance of aryl halide was monitored by TLC) the volatiles were evaporated and the product was purified by flash chromatography on silica gel.

10 obtained in 93 % yield (63.0 mg) (Table 2, Entry 1): ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.04-3.072 (m, 4H), 3.77 (s, 3H), 3.86 (t, 4 H), 6.57-7.00 (m, 4 H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 55.84, 55.59, 67.06, 114.52, 117.83, 150.01.

11 obtained in 95 % yield (73.0 mg) (Table 2, Entry 2): ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.31 (s, 9H), 2.92 (t, J = 4.6Hz, 4H), 3.63 (t, J = 4.7Hz, 4H), 6.85-6.91 (m, 2H), 7.25-7.35 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 31.47, 33.99, 49.59, 67.04, 115.43, 126.00, 142.80, 148.94.

12 obtained in 82 % yield (52.0 mg) (Table 2, Entry 3): ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.45-1.48 (m, 2H), 1.54-1.62 (m, 4H), 2.32 (s, 3H), 2.83-2.91 (m, 4H), 6.89-7.55 (m,

4H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 17.87, 2447, 26.66, 53.37, 118.96, 122.58, 126.41, 130.92, 132.69, 152.96.

13 obtained in 98 % yield (66.0 mg) (Table 2, Entry 5): ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.45-1.55 (m, 2H), 1.69-177 (m, 4H), 2.78-2.82 (m, 4H), 3.77 (s, 3H), 6.81-6.95 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 24.22, 26.16, 52.32, 55.56, 114.33, 118.76, 146.96, 153.56.

14 obtained in 99 % yield (62.0 mg) (Table 2, Entry 6): ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.29 (s, 3H), 3.10-3.19 (m, 4H), 3.85-3.88 (m, 4H), 6.81-6.87 (m, 2H), 7.08-7.11 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.44, 49.95, 67.00, 116.06, 129.58, 129.73, 149.23, 171.92.

16 obtained in 92 % yield (57.0 mg) (Table 2, Entry 8): ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.34 (s, 3H), 2.91-2.94 (m, 4H), 3.85-3.88 (m, 4H), 6.99-7.12 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 17.89, 52.27, 67.49, 118.97, 123.43, 126.68, 131.19, 132.65, 151.31.

17 obtained in 65 % yield (44.0 mg) (Table 2, Entry 9): ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.35 (s, 6H), 3.09-3.12 (m, 4H), 3.79-3.82 (m, 4H), 6.94-7.03 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 19.61, 50.02, 69.00, 125.36, 129.06, 137.00.

18 obtained in 98 % yield (72.0 mg) (Table 2, Entry 10): ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.24 (s, 3H), 3.00 (s, 3H), 4.52 (s, 2H), 6.70-7.28 (m, 9H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.28, 38.67, 57.05, 112.77, 125.82, 126.84, 126.90, 128.55, 129.74, 139.30, 147.86.

19 obtained in 76 % yield (71.0 mg) (Table 2, Entry 11): ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.16-1.18 (m, 12H), 2.26 (s, 3H), 2.94-2.98 (m, 2H), 5.06 (m, 1H, N<u>H</u>), 6.42-7.35 (m, 7H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 20.46, 23.89, 28.21, 113.09, 123.82, 126.84, 127.00, 129.74, 135.60, 145.84, 147.40.

20 obtained in 96 % yield (74.0 mg) (Scheme 9): ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.93-1.00 (m, 6H), 1.31-1.44 (m, 4H), 1.53-1.63 (m, 4H), 2.27 (s, 3H), 3.24-3.28 (m, 4H), 6.60-6.63 (m, 2H), 7.03-7.06 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 14.08, 20.18, 20.44, 29.50, 51.04, 112.23, 124.36, 129.73, 146.26.

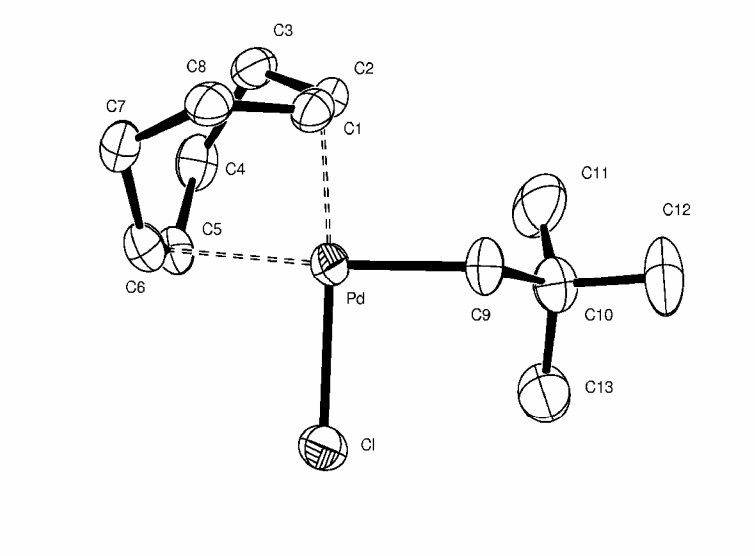


Table 1. Crystal data and structure refinement for [Pd(1,5-COD) (neopentyl)Cl], **1**

Identification code	jun1505	
Empirical formula	C13 H23 Cl Pd	
Formula weight	321.16	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$ (No.14)	
Unit cell dimensions	a = 6.4359(5) Å	α= 90°.
	b = 12.0616(10) Å	β= 96.456(4)°.
	c = 17.4155(14) Å	γ = 90°.
Volume	1343.34(19) $Å^3$	
Z	4	
Density (calculated)	1.59 Mg/m^3	
Absorption coefficient	1.55 mm^{-1}	

F(000)	656
Crystal size	0.10 x 0.10 x 0.05 mm^3
Theta range for data collection	3.52 to 22.97°.
Index ranges	-6<=h<=7, -13<=k<=12, -19<=l<=17
Reflections collected	6834
Independent reflections	1843 [R(int) = 0.088]
Reflections with I>2sigma(I)	1451
Completeness to theta = 22.97°	99.7 %
Tmax. and Tmin.	0.9045 and 0.8147
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1843 / 0 / 136
Goodness-of-fit on F^2	1.105
Final R indices [I>2sigma(I)]	R1 = 0.060, wR2 = 0.134
R indices (all data)	R1 = 0.082, wR2 = 0.148
Largest diff. peak and hole	1.33 and -0.87 e.$Å^{-3}$ (near Pd)

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jun1505. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd	1346(1)	3682(1)	3584(1)	31(1)
Cl	-1090(4)	2373(2)	3070(2)	41(1)
C(1)	2216(15)	5289(7)	4056(5)	35(2)
C(2)	4007(14)	4743(7)	3929(5)	31(2)
C(3)	5334(14)	4960(8)	3273(5)	37(2)
C(4)	4614(15)	4324(8)	2508(6)	39(2)
C(5)	2319(14)	4151(8)	2335(5)	37(2)
C(6)	797(15)	4867(8)	2431(5)	35(2)
C(7)	1152(15)	6039(8)	2700(6)	38(2)
C(8)	1074(15)	6186(7)	3561(5)	38(2)
C(9)	1423(15)	2990(8)	4674(5)	38(2)
C(10)	2774(15)	1961(8)	4864(6)	41(2)
C(11)	5066(18)	2155(10)	4747(8)	65(4)
C(12)	2610(20)	1684(10)	5714(6)	69(4)
C(13)	1990(20)	948(9)	4389(7)	59(3)

Table 3. Bond lengths [Å] and angles [°] for jun1505.

Pd-M(1)	2.049(8)
Pd-C(9)	2.070(9)
Pd-C(1)	2.155(8)
Pd-C(2)	2.168(8)
Pd-Cl	2.332(2)
Pd-M(2)	2.335(9)
Pd-C(5)	2.398(10)
Pd-C(6)	2.457(9)
C(1)-C(2)	1.367(12)
C(1)-C(8)	1.520(13)
C(2)-C(3)	1.524(13)
C(3)-C(4)	1.561(13)
C(4)-C(5)	1.489(13)
C(5)-C(6)	1.330(13)
C(6)-C(7)	1.499(13)
C(7)-C(8)	1.515(13)
C(9)-C(10)	1.529(13)
C(10)-C(11)	1.530(15)
C(10)-C(13)	1.529(15)
C(10)-C(12)	1.533(15)

M(1)-Pd-C(9)	92.4(3)
M(1)-Pd-Cl	170.8(3)
C(9)-Pd-Cl	91.4(3)
M(1)-Pd-M(2)	83.7(3)
C(9)-Pd-M(2)	175.1(3)
Cl-Pd-M(2)	92.8(3)
C(2)-C(1)-C(8)	127.8(9)
C(2)-C(1)-Pd	72.1(5)
C(8)-C(1)-Pd	109.6(6)
C(1)-C(2)-C(3)	126.3(8)
C(1)-C(2)-Pd	71.0(5)
C(3)-C(2)-Pd	112.7(6)
C(2)-C(3)-C(4)	114.7(7)
C(5)-C(4)-C(3)	115.7(8)
C(6)-C(5)-C(4)	127.7(9)
C(6)-C(5)-Pd	76.6(6)
C(4)-C(5)-Pd	101.8(6)
C(5)-C(6)-C(7)	124.3(9)
C(5)-C(6)-Pd	71.7(6)
C(7)-C(6)-Pd	106.9(6)
C(6)-C(7)-C(8)	113.4(8)
C(7)-C(8)-C(1)	114.2(8)
C(10)-C(9)-Pd	118.7(7)

C(11)-C(10)-C(9)	112.3(9)
C(11)-C(10)-C(13)	108.3(9)
C(9)-C(10)-C(13)	112.7(8)
C(11)-C(10)-C(12)	109.6(9)
C(9)-C(10)-C(12)	106.6(8)
C(13)-C(10)-C(12)	107.1(9)

M(1) and M(2) are the mid-points of the C(1)-C(2) and C(5)-C(6) bonds.

```
Least-squares planes (x,y,z in crystal coordinates) and deviations from
them
 (* indicates atom used to define plane)

 - 5.1975 (0.0024) x + 6.8700 (0.0102) y + 4.2282 (0.0340) z = 3.3998
(0.0074)

 *    0.0957 (0.0022)  Cl_a
 *   -0.1095 (0.0025)  C9_a
 *    0.1175 (0.0027)  M1_b
 *   -0.1037 (0.0023)  M2_b
     -0.0546 (0.0027)  Pd
      0.7970 (0.0097)  C1_a
     -0.5628 (0.0095)  C2_a
     -0.7656 (0.0100)  C5_a
      0.5576 (0.0096)  C6_a
     -0.1095 (0.0025)  C9_a

 Rms deviation of fitted atoms =   0.1069
```

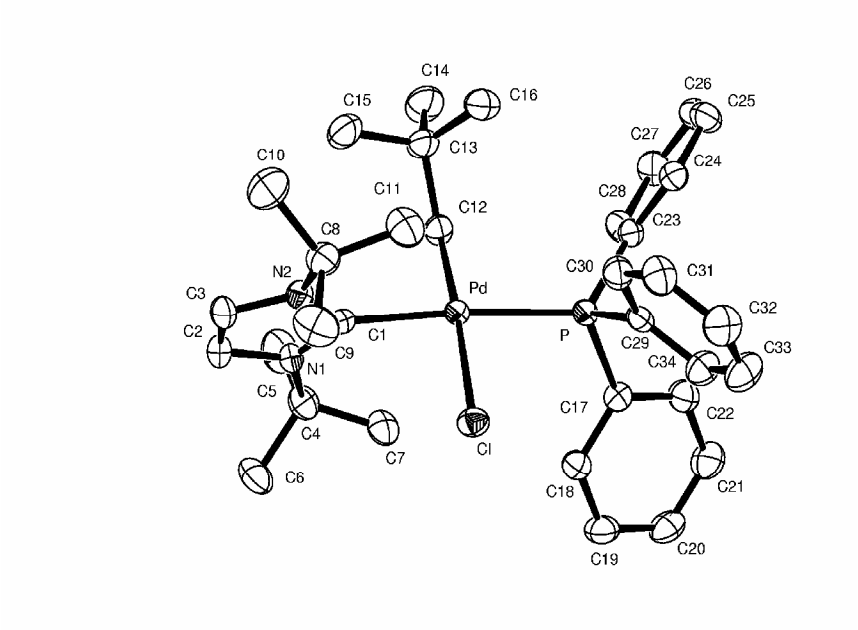


Table 1. Crystal data and structure refinement for $[Pd(I^tBu)(PPh_3)(neopentyl)(Cl)]$, **5**

Identification code	nov205	
Empirical formula	C34 H46 Cl N2 P Pd . 2(C7 H8)	
Formula weight	839.82	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$ (No.19)	
Unit cell dimensions	a = 12.3007(2) Å	α= 90°.
	b = 18.7039(2) Å	β= 90°.
	c = 19.5365(3) Å	γ = 90°.
Volume	4494.78(11) $Å^3$	
Z	4	

Density (calculated)	1.24 Mg/m^3
Absorption coefficient	0.54 mm^{-1}
F(000)	1768
Crystal size	0.3 x 0.1 x 0.1 mm^3
Theta range for data collection	3.43 to 26.01°.
Index ranges	-15<=h<=14, -23<=k<=23, -24<=l<=24
Reflections collected	69469
Independent reflections	8839 [R(int) = 0.064]
Reflections with I>2sigma(I)	8026
Completeness to theta = 26.01°	99.7 %
Tmax. and Tmin.	0.955 and 0.869
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8839 / 0 / 478
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.031, wR2 = 0.060
R indices (all data)	R1 = 0.040, wR2 = 0.063
Absolute structure parameter	-0.019(18)
Largest diff. peak and hole	0.34 and -0.24 $e.Å^{-3}$

Data collection KappaCCD , Program package WinGX , Abs correction MULTISCAN

Refinement using SHELXL-97 , Drawing using ORTEP-3 for Windows

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for nov205. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd	4138(1)	5868(1)	4175(1)	21(1)
Cl	3531(1)	6248(1)	5316(1)	29(1)
P	2425(1)	5391(1)	3974(1)	22(1)
N(1)	5945(2)	7021(1)	4179(1)	26(1)
N(2)	6442(2)	6115(1)	4794(1)	28(1)
C(1)	5605(2)	6359(1)	4395(1)	24(1)
C(2)	6977(3)	7160(2)	4425(2)	35(1)
C(3)	7283(3)	6607(2)	4802(2)	36(1)
C(4)	5360(3)	7578(2)	3754(2)	33(1)
C(5)	5837(3)	7564(2)	3033(2)	49(1)
C(6)	5561(3)	8315(1)	4080(2)	44(1)
C(7)	4147(3)	7455(1)	3745(2)	34(1)
C(8)	6509(3)	5479(2)	5268(2)	34(1)
C(9)	6348(3)	5754(2)	6000(2)	51(1)
C(10)	7633(3)	5141(2)	5192(2)	55(1)
C(11)	5652(3)	4920(2)	5114(2)	41(1)
C(12)	4647(2)	5657(1)	3175(1)	27(1)
C(13)	5404(3)	5033(2)	2982(2)	34(1)

C(14)	5442(3)	5004(2)	2194(2)	49(1)
C(15)	6567(3)	5158(2)	3240(2)	45(1)
C(16)	4983(3)	4311(2)	3233(2)	42(1)
C(17)	1350(2)	6062(1)	3853(1)	25(1)
C(18)	1490(2)	6741(1)	4133(2)	29(1)
C(19)	668(3)	7247(2)	4086(2)	37(1)
C(20)	-293(3)	7085(2)	3756(2)	39(1)
C(21)	-435(3)	6411(2)	3475(2)	43(1)
C(22)	379(2)	5909(2)	3523(2)	36(1)
C(23)	2161(2)	4785(1)	3256(1)	24(1)
C(24)	2049(2)	4051(2)	3348(1)	28(1)
C(25)	1868(3)	3604(2)	2797(2)	35(1)
C(26)	1804(3)	3880(2)	2145(2)	37(1)
C(27)	1918(3)	4605(2)	2040(2)	36(1)
C(28)	2102(3)	5056(2)	2593(2)	33(1)
C(29)	1940(2)	4879(1)	4713(1)	24(1)
C(30)	2664(3)	4424(2)	5047(2)	31(1)
C(31)	2328(3)	4028(2)	5605(2)	38(1)
C(32)	1290(3)	4087(2)	5845(2)	43(1)
C(33)	569(3)	4537(2)	5524(2)	43(1)
C(34)	890(3)	4932(2)	4959(1)	35(1)
C(1S)	2608(5)	2158(3)	4117(3)	83(1)
C(2S)	1605(5)	2382(2)	4338(2)	79(2)

C(3S)	658(6)	2088(3)	4020(3)	92(2)
C(4S)	810(7)	1592(3)	3499(3)	94(2)
C(5S)	1847(9)	1400(4)	3324(3)	119(3)
C(6S)	2713(9)	1674(4)	3624(3)	131(3)
C(7S)	3590(7)	2450(4)	4425(4)	166(3)
C(8S)	8430(4)	3398(2)	3465(3)	80(2)
C(9S)	7504(4)	3219(2)	3810(2)	70(1)
C(10S)	6824(4)	2706(2)	3567(3)	69(1)
C(11S)	7085(4)	2337(2)	2974(2)	72(1)
C(12S)	8002(5)	2503(3)	2635(2)	84(2)
C(13S)	8669(4)	3037(3)	2868(3)	86(2)
C(14S)	9156(5)	3970(3)	3729(4)	145(3)

Table 3. Bond lengths [Å] and angles [°] for nov205.

Pd-C(1)	2.070(3)
Pd-C(12)	2.090(3)
Pd-P	2.3211(8)
Pd-Cl	2.4554(7)
P-C(29)	1.831(3)
P-C(23)	1.832(3)
P-C(17)	1.838(3)
N(1)-C(1)	1.375(3)
N(1)-C(2)	1.382(4)
N(1)-C(4)	1.514(4)
N(2)-C(1)	1.370(3)
N(2)-C(3)	1.386(4)
N(2)-C(8)	1.509(4)
C(2)-C(3)	1.323(4)
C(4)-C(7)	1.509(5)
C(4)-C(5)	1.527(4)
C(4)-C(6)	1.539(4)
C(8)-C(11)	1.515(4)
C(8)-C(10)	1.528(5)
C(8)-C(9)	1.531(4)
C(12)-C(13)	1.539(4)

C(13)-C(16)	1.528(4)
C(13)-C(15)	1.535(5)
C(13)-C(14)	1.541(4)
C(17)-C(22)	1.388(4)
C(17)-C(18)	1.394(4)
C(18)-C(19)	1.387(4)
C(19)-C(20)	1.380(5)
C(20)-C(21)	1.386(5)
C(21)-C(22)	1.376(4)
C(23)-C(28)	1.392(4)
C(23)-C(24)	1.393(4)
C(24)-C(25)	1.381(4)
C(25)-C(26)	1.376(4)
C(26)-C(27)	1.379(4)
C(27)-C(28)	1.388(4)
C(29)-C(34)	1.382(4)
C(29)-C(30)	1.394(4)
C(30)-C(31)	1.382(4)
C(31)-C(32)	1.364(4)
C(32)-C(33)	1.375(4)
C(33)-C(34)	1.385(4)
C(1S)-C(6S)	1.328(8)
C(1S)-C(2S)	1.374(7)

C(1S)-C(7S)	1.455(9)
C(2S)-C(3S)	1.429(7)
C(3S)-C(4S)	1.391(7)
C(4S)-C(5S)	1.368(10)
C(5S)-C(6S)	1.319(11)
C(8S)-C(9S)	1.365(7)
C(8S)-C(13S)	1.380(7)
C(8S)-C(14S)	1.486(6)
C(9S)-C(10S)	1.358(6)
C(10S)-C(11S)	1.387(6)
C(11S)-C(12S)	1.344(6)
C(12S)-C(13S)	1.370(6)

C(1)-Pd-C(12)	90.92(11)
C(1)-Pd-P	175.49(7)
C(12)-Pd-P	92.36(8)
C(1)-Pd-Cl	87.04(7)
C(12)-Pd-Cl	174.01(8)
P-Pd-Cl	89.38(2)
C(29)-P-C(23)	102.85(12)
C(29)-P-C(17)	102.99(13)
C(23)-P-C(17)	101.29(13)
C(29)-P-Pd	111.28(9)

C(23)-P-Pd	121.87(10)
C(17)-P-Pd	114.34(9)
C(1)-N(1)-C(2)	110.0(2)
C(1)-N(1)-C(4)	130.1(2)
C(2)-N(1)-C(4)	119.9(2)
C(1)-N(2)-C(3)	110.2(2)
C(1)-N(2)-C(8)	130.7(2)
C(3)-N(2)-C(8)	118.5(2)
N(2)-C(1)-N(1)	104.3(2)
N(2)-C(1)-Pd	128.76(19)
N(1)-C(1)-Pd	126.98(19)
C(3)-C(2)-N(1)	108.0(3)
C(2)-C(3)-N(2)	107.5(3)
C(7)-C(4)-N(1)	111.8(2)
C(7)-C(4)-C(5)	111.5(3)
N(1)-C(4)-C(5)	108.2(3)
C(7)-C(4)-C(6)	107.4(3)
N(1)-C(4)-C(6)	108.2(2)
C(5)-C(4)-C(6)	109.6(2)
N(2)-C(8)-C(11)	112.6(2)
N(2)-C(8)-C(10)	108.4(3)
C(11)-C(8)-C(10)	108.9(3)
N(2)-C(8)-C(9)	107.5(2)

C(11)-C(8)-C(9)	109.2(3)
C(10)-C(8)-C(9)	110.3(3)
C(13)-C(12)-Pd	123.67(19)
C(16)-C(13)-C(15)	110.1(3)
C(16)-C(13)-C(12)	112.7(3)
C(15)-C(13)-C(12)	111.6(3)
C(16)-C(13)-C(14)	107.5(3)
C(15)-C(13)-C(14)	107.8(3)
C(12)-C(13)-C(14)	106.9(3)
C(22)-C(17)-C(18)	118.4(3)
C(22)-C(17)-P	122.6(2)
C(18)-C(17)-P	118.9(2)
C(19)-C(18)-C(17)	120.4(3)
C(20)-C(19)-C(18)	120.4(3)
C(19)-C(20)-C(21)	119.5(3)
C(22)-C(21)-C(20)	120.1(3)
C(21)-C(22)-C(17)	121.2(3)
C(28)-C(23)-C(24)	118.2(3)
C(28)-C(23)-P	119.8(2)
C(24)-C(23)-P	121.9(2)
C(25)-C(24)-C(23)	120.8(3)
C(26)-C(25)-C(24)	120.2(3)
C(25)-C(26)-C(27)	120.0(3)

C(26)-C(27)-C(28)	119.9(3)
C(27)-C(28)-C(23)	120.8(3)
C(34)-C(29)-C(30)	118.5(3)
C(34)-C(29)-P	122.8(2)
C(30)-C(29)-P	118.7(2)
C(31)-C(30)-C(29)	120.4(3)
C(32)-C(31)-C(30)	120.5(3)
C(31)-C(32)-C(33)	119.8(3)
C(32)-C(33)-C(34)	120.4(3)
C(29)-C(34)-C(33)	120.4(3)
C(6S)-C(1S)-C(2S)	121.6(7)
C(6S)-C(1S)-C(7S)	118.4(7)
C(2S)-C(1S)-C(7S)	120.0(6)
C(1S)-C(2S)-C(3S)	118.5(5)
C(4S)-C(3S)-C(2S)	117.7(6)
C(5S)-C(4S)-C(3S)	118.9(7)
C(6S)-C(5S)-C(4S)	122.7(7)
C(5S)-C(6S)-C(1S)	120.5(8)
C(9S)-C(8S)-C(13S)	118.3(4)
C(9S)-C(8S)-C(14S)	120.5(5)
C(13S)-C(8S)-C(14S)	121.2(5)
C(10S)-C(9S)-C(8S)	121.0(5)
C(9S)-C(10S)-C(11S)	120.1(5)

C(12S)-C(11S)-C(10S)	119.3(4)
C(11S)-C(12S)-C(13S)	120.5(5)
C(12S)-C(13S)-C(8S)	120.7(5)

```
 Least-squares planes (x,y,z in crystal coordinates) and deviations
from them
 (* indicates atom used to define plane)

 - 4.1139 (0.0069) x + 16.4132 (0.0052) y - 6.7136 (0.0108) z = 5.1928
(0.0079)

 *   -0.0100 (0.0010)  P
 *    0.0416 (0.0010)  Cl
 *   -0.0128 (0.0011)  C1
 *    0.0481 (0.0011)  C12
 *   -0.0669 (0.0009)  Pd

 Rms deviation of fitted atoms =   0.0419


 - 4.9657 (0.0165) x + 7.9989 (0.0238) y + 15.8009 (0.0161) z = 9.2587
(0.0211)

 Angle to previous plane (with approximate esd) = 76.56 ( 0.08 )

 *   -0.0110 (0.0016)  C1
 *   -0.0042 (0.0018)  C2
 *   -0.0029 (0.0018)  C3
 *    0.0094 (0.0017)  N1
 *    0.0086 (0.0017)  N2

 Rms deviation of fitted atoms =   0.0079
```